Statistical Aspects of Quantum Computing

Yazhen Wang

Department of Statistics

University of Wisconsin-Madison

http://www.stat.wisc.edu/~yzwang

Near-term Applications of Quantum Computing

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Outline

- Statistical learning with quantum annealing
- Statistical analysis of quantum computing data

Statistics and Optimization

MLE/M-estimation, Non-parametric smoothing, $\cdots$

- Stochastic optimization problem: $\min_\theta \mathcal{L}(\theta; \mathbf{X}_n) = \frac{1}{n}\sum_{i=1}^{n} \ell(\theta; X_i)$

- Minimization solution gives an estimator or a classifier.
  Examples : $\ell(\theta; X_i) = \log pdf$; residual square sum / loss + penalty

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Take $g(\theta) = E[\mathcal{L}(\theta; \mathbf{X}_n)] = E[\ell(\theta; X_1)]$

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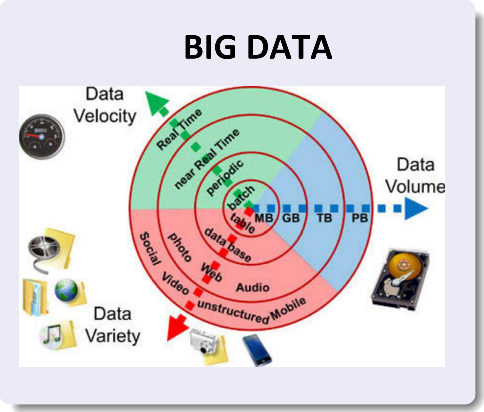
Goals: Use data $\mathbf{X}_n$ to do the following

(i) Evaluate estimators/classifiers (minimization solutions) **Computing**
(ii) Statistical study of estimators/classifiers – **Inference**

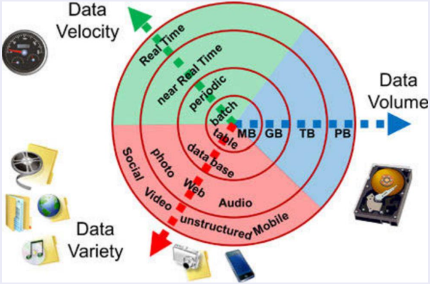
Computer Power Demand

Computer Power Demand

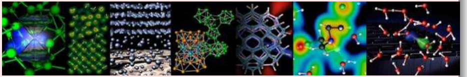


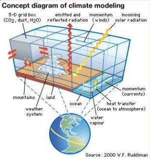
Computer Power Demand

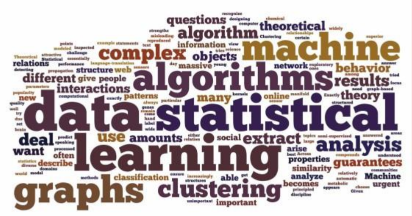
BIG DATA



Scientific Studies and Computational Applications







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Machine learning and compressed sensing

• Matrix completion, matrix factorization, tensor decomposition, phase retrieval, neural network.

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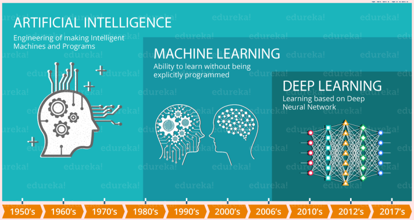

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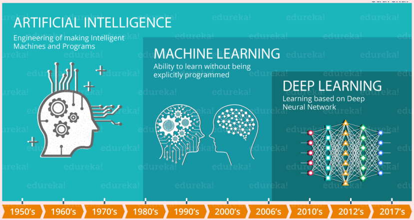
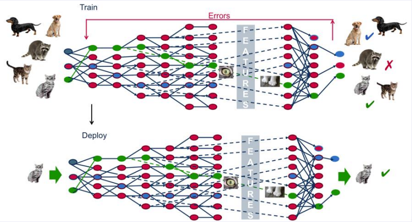


Dog vs cat



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Neural network: Layers in a chain structure

Each layer is a function of the layer preceded it.

Layer j: $h_j = g_j(a_j h_{j-1} + b_j)$, $(a_j, b_j) =$ weights,

$g_j =$ activation function (sigmoid, softmax or rectifier)

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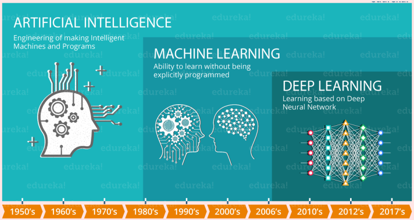

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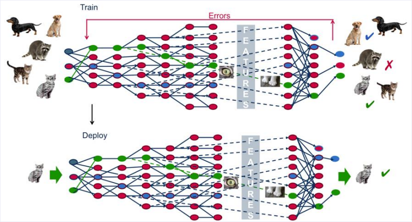

Gradient Descent Alorithms: Solve $\min_\theta g(\theta)$

Gradient descent algorithm

- Start at initial value x_0,
  $x_k = x_{k-1} - \delta \nabla g(x_{k-1}), \;\; \delta =$ learning rate, $\nabla =$ derivative operator

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Accelerated Gradient descent algorithm (Nesterov)

- Start at initial values x_0 and $y_0 = x_0$,

$$x_k = y_{k-1} - \delta \nabla g(y_{k-1}), \qquad y_k = x_k + \frac{k-1}{k+2}(x_k - x_{k-1})$$

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Continuous curve X_t to approximate discrete $\{x_k : k \geq 0\}$

Differential equation: $\dot{X}_t + \nabla g(X_t) = 0$, $\dot{X}_t =$ derivative $= \dfrac{dX_t}{dt}$

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Convergence to the minimization solution at rate= $1/k$ or $1/t$ $(\uparrow)$

as $t, k \to \infty$. For the ccelerated case: Rate = $1/k^2$ or $1/t^2 (\downarrow)$

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Stochastic optimization: $\min_\theta \mathcal{L}(\theta; \mathbf{X}_n)$, $\mathbf{X}_n = (X_1, \cdots, X_n)$

- Gradient descent algorithm to compute x_k iteratively

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BigData: expensive to evaluate all $\nabla \ell(\theta; X_i)$ at each iteration

- Replace $\nabla \mathcal{L}(\theta; \mathbf{X}_n)$ by

$$\nabla \hat{\mathcal{L}}^m(\theta; \mathbf{X}^*_m) = \frac{1}{m} \sum_{j=1}^{m} \nabla \ell(\theta; X^*_j), \qquad m \ll n$$

$\mathbf{X}^*_m = (X^*_1, \cdots, X^*_m)$= subsample of $\mathbf{X}_n$ (minibatch or bootstrap sample).

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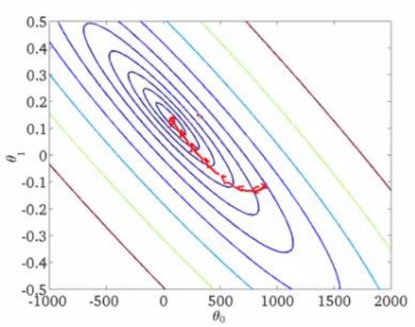
X_t^* obeys stochastic differential equation.

Gradient Descent vs Stochastic Gradient Descent

Gradient Descent



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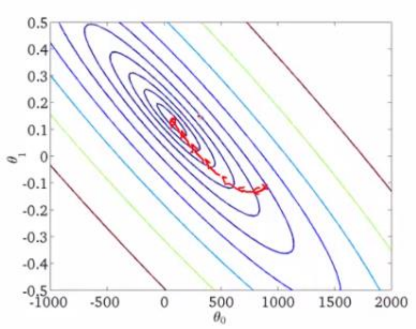

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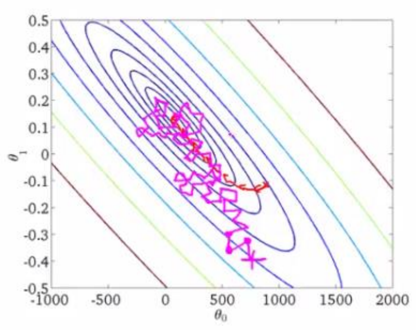

Statistical Analysis of Gradient Descent (Wang, 2017)

Continuous curve model

Stochastic differential equation:

$$dX_t^* + \nabla g(X_t^*)dt + \sigma(X_t^*)dW_t = 0$$

W_t = Brownian motion

For the accelerated case:

2nd order stochastic differential equation

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and their asymptotic distribution

as $m, n \to \infty$ via stochastic differential equations

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Example $X_i = (U_i, V_i)$, $i = 1, \cdots, n = 10000$

$$V_i = U_i\theta + \varepsilon_i, \quad U_i \sim i.i.d.\text{bivariate}N(0, \Sigma), \varepsilon_i \sim i.i.d.N(0, \tau^2)$$

$\ell(\theta; X_i) = (V_i - U_i\theta)^2$, $m = 200$, true $\theta = (0, 0)$.

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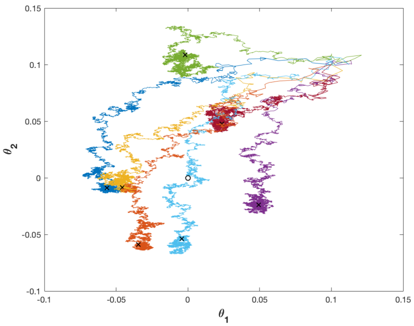

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Deep Learning

Boltzmann Machine (BM) on graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$

- $$P(\mathbf{s}) = \frac{\exp[-E(\mathbf{s})]}{Z}, \quad Z = \sum_{\mathbf{s}} \exp[-E(\mathbf{s})]$$
- Energy
$$E(\mathbf{s}) = -\sum_{(i,j)\in\mathcal{E}} W_{ij} s_i s_j - \sum_{i\in\mathcal{V}} b_i s_i, \quad \mathbf{s} = (s_1, \cdots, s_{|\mathcal{V}|}) \in \{-1, 1\}^{|\mathcal{V}|}$$

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Take $\mathbf{s} = (\mathbf{v}, \boldsymbol{h})$

$\mathbf{v} = (\mathbf{v_1}, \cdots, \mathbf{v_n})$: visible nodes (observed variables)

$\boldsymbol{h} = (h_1, \cdots, h_m)$: hidden nodes (latent variables).

Boltzmann distribution models data $\mathbf{v}$:

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Learning

Use training data $\mathbf{v}$ to learn model parameters W_{ij} & b_i.

Restricted Boltzmann Machine (RBM)

Bipartite undirected graph $\mathcal{G}$

Connections between hidden layer
and visible layer
but not within each layer

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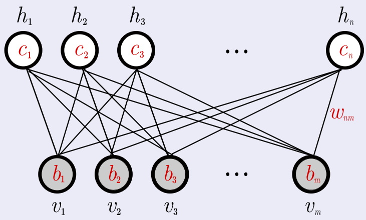
Model

Variables in visible layer:
$\mathbf{v} = (v_1, \cdots, v_n)$,
Variables in hidden layer:
$\boldsymbol{h} = (h_1, \cdots, h_m)$

$$P(\mathbf{v}, \boldsymbol{h}) = \exp\{-E(\mathbf{v}, \boldsymbol{h})\}/Z$$



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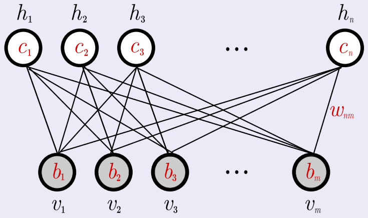

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$$E(\mathbf{v}, \boldsymbol{h}) = -\sum_{i=1}^{n}\sum_{j=1}^{m} w_{ij} v_i h_j - \sum_{i=1}^{n} b_i v_i - \sum_{j=1}^{m} c_j h_j$$

Deep Neural Network: Restricted Boltzmann Machine

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Conditional independence within each layer given the others

$$P(\boldsymbol{h}|\mathbf{v}) = \prod_{j=1}^{m} P(h_j|\mathbf{v}), \quad P(\mathbf{v}|\boldsymbol{h}) = \prod_{i=1}^{n} P(v_i|\boldsymbol{h})$$

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Sigmoid activation function for forward and backward conditional probabilities: sigmoid$(x) = 1/[1 + e^{-x}]$

$$P(h_j = 1|\mathbf{v}) = \text{sigmoid}\left(\sum_{i=1}^{n} w_{ij} v_i + c_j\right)$$

$$P(v_i = 1|\boldsymbol{h}) = \text{sigmoid}\left(\sum_{j=1}^{n} w_{ij} h_j + b_i\right)$$

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Parameter updates with learning rate η

$$w_{ij}^{(t+1)} = w_{ij}^{t} + \eta \frac{\partial \log P}{\partial w_{ij}}$$

$$b_i^{(t+1)} = b_i^{t} + \eta \frac{\partial \log P}{\partial b_i}, \quad c_j^{(t+1)} = c_j^{t} + \eta \frac{\partial \log P}{\partial c_j}$$

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Gradient

$$\frac{\partial \log P}{\partial w_{ij}} = \langle v_i h_j \rangle_{\text{data}} - \langle v_i h_j \rangle_{\text{model}}$$

$$\frac{\partial \log P}{\partial b_i} = \langle v_i \rangle_{\text{data}} - \langle v_i \rangle_{\text{model}}, \quad \frac{\partial \log P}{\partial c_j} = \langle h_j \rangle_{\text{data}} - \langle h_j \rangle_{\text{model}}$$

- $\langle v_i h_j \rangle_{\text{data}}$: the clamped expectation with **v** fixed

Bottleneck : $$\langle v_i h_j \rangle_{\text{model}} = \sum_{\mathbf{v}, \boldsymbol{h}} v_i h_j P(\mathbf{v}, \boldsymbol{h})$$

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Markov Chain Monte Carlo (MCMC)

Metropolis-Hastings algorithm/Gibbs sampler

Sample from Boltzmann distribution

$$P(\mathbf{s}) = \frac{\exp[-H_{Ising}(\mathbf{s})/T]}{Z_T}, Z_T = \sum_{\mathbf{s}} \exp\left[-\frac{H_{Ising}(\mathbf{s})}{T}\right], T = \text{temperature}$$

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Simulated annealing: Thermal Fluctuation

Slowly lower the temperature to reduce the escape probability of trapping in local minima,

$$\text{Annealing schedule}: T_i \propto \frac{1}{i+1} \text{ or } \frac{1}{\log(i+1)}$$

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BigData

Issues: not easy for parallel computing; very hard to scale-up!

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Classical optimization: Min$\{H_{Ising}(\mathbf{s}) : \mathbf{s} \in \{-1, 1\}^N\}$

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Find a target quantum system with Hamiltonian $H(1)$ whose energies match $H_{Ising}(\mathbf{s})$: $H(1) = \text{diag}\{H_{Ising}(\mathbf{s}_1,) \cdots, H_{Ising}(\mathbf{s}_{2^N})\}$.

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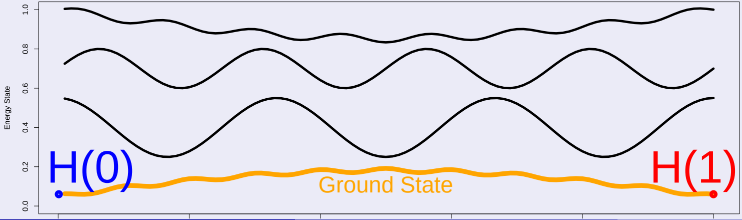
QA: Engineer $H(0)$ in its lowest energy state and gradually move

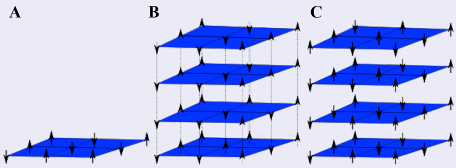
$H(0) \longrightarrow H(1)$



Simulated Quantum Annealing (SQA)

Spin glass in transverse field

$$H = \mathbf{A(t)H_X} + \mathbf{B(t)H_{Ising}}, \quad \text{two parts non-commuting}$$



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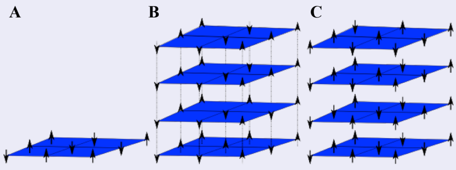

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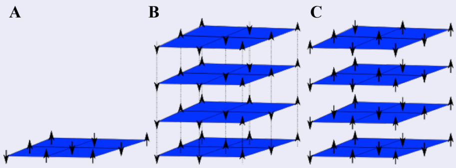

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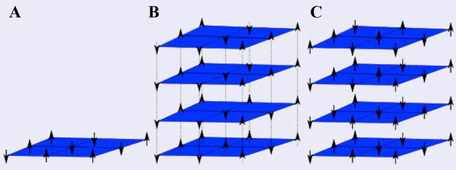
Quantum Monte Carlo

H_{2+1}: a collection of 2-dimensional classical Ising systems, that can be simulated by MCMC with moves in both directions



SSSV Annealing Model

Magnet i points in direction with angle θ_i w.r.t. $\vec{z}$-axis in the xz plane, an external magnetic field with intensity $A(t)$ pointing in the $\vec{x}$-axis,

Hamiltonian, J_{ij} = coupling of magnets θ_i and θ_j,

$$H(t) = -A(t)\sum_{i=1}^{N}\sin\theta_i - B(t)\sum_{1\le i<j\le N} J_{ij}\cos\theta_i\cos\theta_j$$

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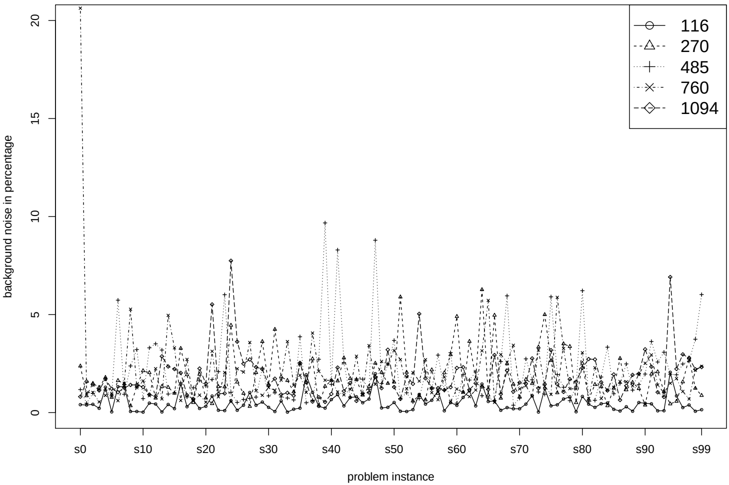
Use the converted states to evaluate $H_{Ising}(\mathbf{s})$ and find its minimizer

DW Signal vs Background Noise



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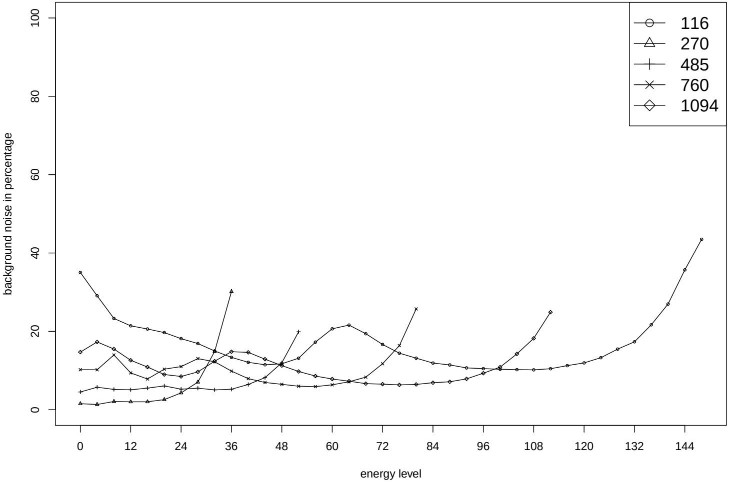
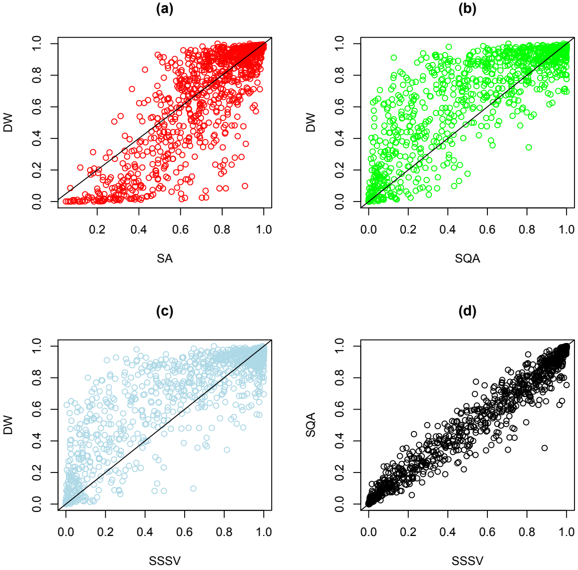


Correlation of Ground State Success Probability Data



Multiple Statistical Tests

For the r-th instance, repeat m times of annealing, let $\hat{p}_{0rm}$ be DW success frequency out of m repetitions and $\hat{q}_{\ell rm}$, $\ell = 1, 2, 3$, the success frequencies for SA, SQA & SSSV

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Asymptotic distribution under H_{0r}

As $m, n \to \infty$, if $\log n/m \to 0$, then

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p-values & FDR

H_{0r} vs H_{ar} : p-value = $P(\chi^2_1 \geq T_{r\ell})$ p-value = $P(\chi^2_1 \geq T^*_{r\ell})$

Goodness-of-fit test

$H_0 : p_{0r\infty} = q_{\ell r\infty}$ for all $1 \leq r \leq n$ vs $H_a : p_{0r\infty} \neq q_{\ell r\infty}$ for some r

$$U_\ell = (2n)^{-1/2} \sum_{r=1}^{n} (T_{r\ell} - n) \quad U_\ell^* = (2n)^{-1/2} \sum_{r=1}^{n} (T_{r\ell} - n)$$

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Asymptotic distribution under H_0 as $m, n \to \infty$

$$U_\ell \to N(0,1) \quad U_\ell^* \to N(0,1)$$

Conditions

(1) $\sqrt{n}/m \to 0$.

(2) $p_{0r\infty} = q_{\ell r\infty}$=true success probability for method ℓ with the r-th instance are bounded away from 0 and 1.

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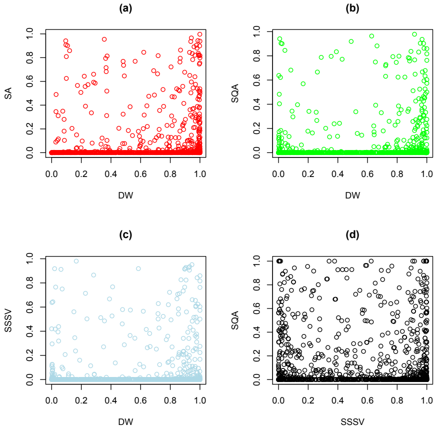

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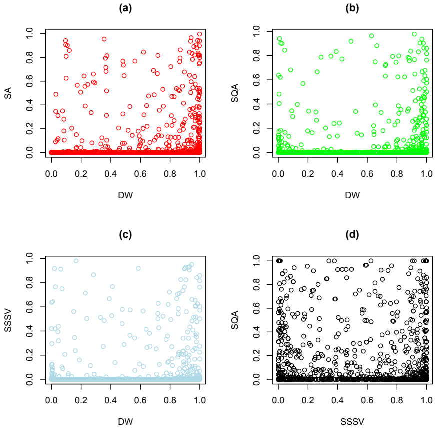

p-values

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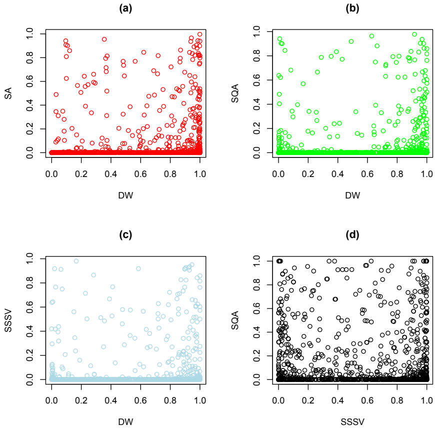

p-values

FDR

q-value = essentially zero

Goodness-of-fit-test

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SQA vs DW

p-values = 0

Goodness-of-fit-test

SQA vs DW

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SSSV vs DW

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Reject null hypothesis

all p-values $\leq 3.87 \times 10^{-6}$

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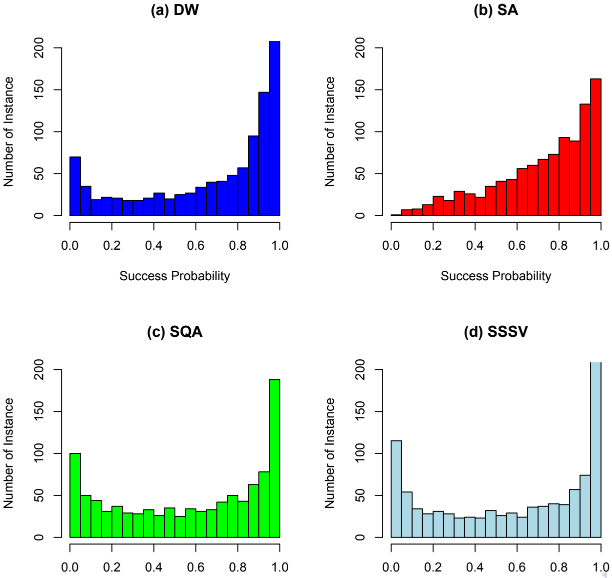
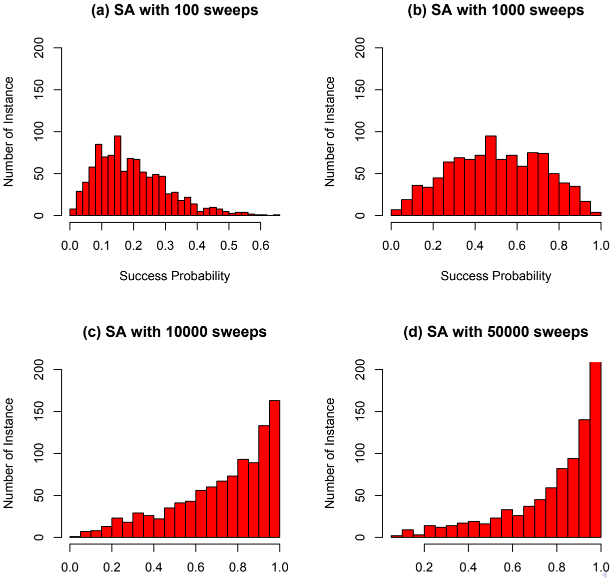
Conclusion: Overwhelming rejection

Overwhelming evidence to reject that DW is statistically consistent with SQA or SSSV in terms of ground state success probability

Histogram of Ground State Success Probability Data

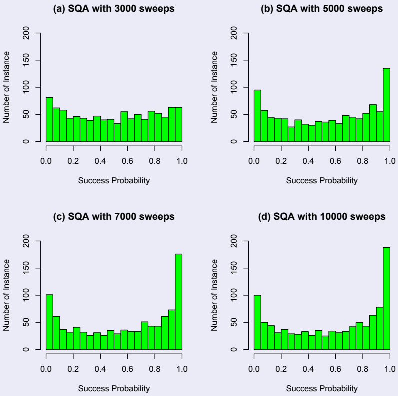


SA Histograms for different annealing times



SQA Histograms

Various annealing times



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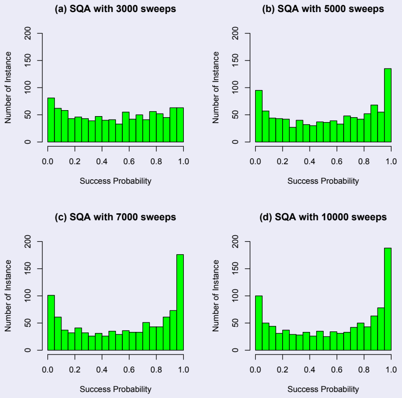
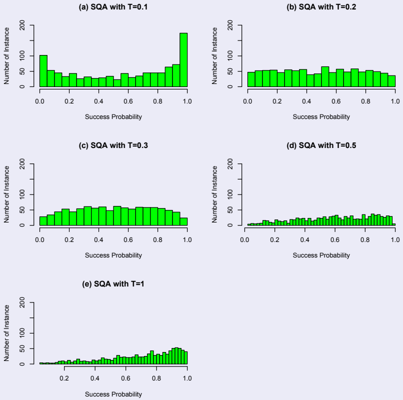


Various temperatures



SSSV Histograms

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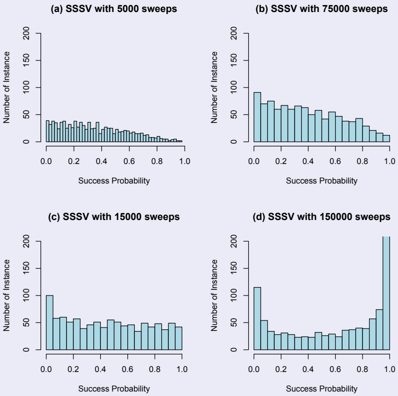

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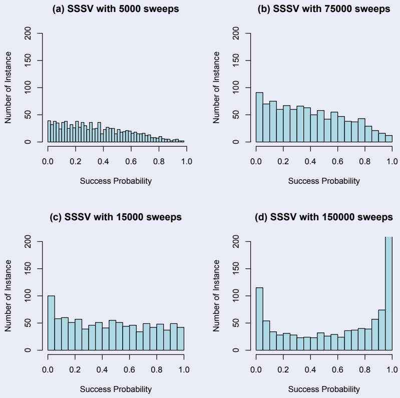

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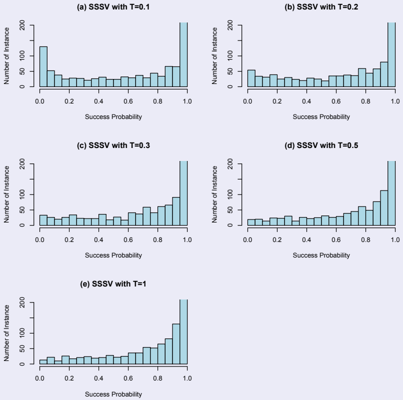

DIP Test for Shape Patterns

$$DIP(F_n) = \max_{0 \le p \le 1} |F_n(p) - \hat{F}_n(p)|$$

F_n=empirical DF, $\hat{F}_n$= DF estimator under unimodality or U-shape

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Unimodality (including monotone)

DW: no

SA: yes

SQA: no

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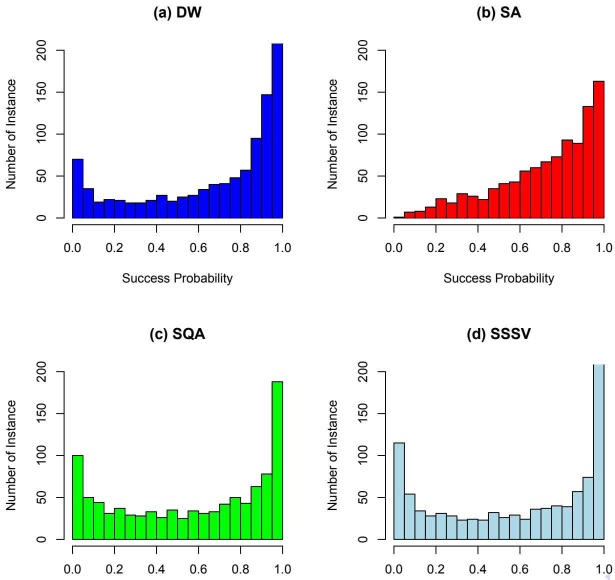
Histogram of Success Probability



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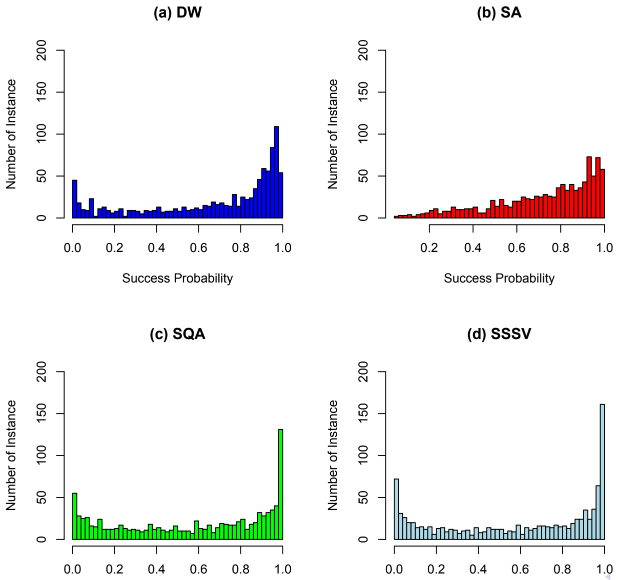


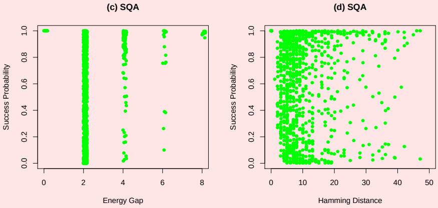
Shape Pattern Analysis by Regression

Covariates

Energy gap & Hamming distance between ground state and 1st excited state

Shape Pattern Analysis by Regression

SQA



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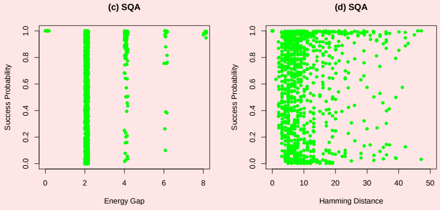

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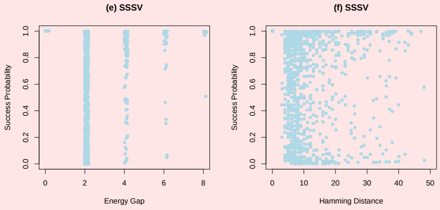

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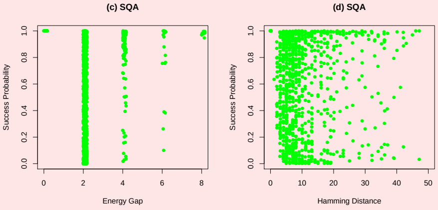
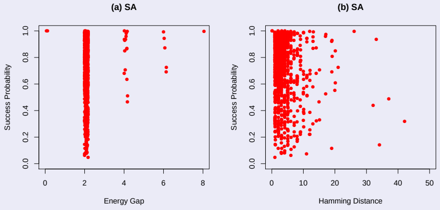


SA



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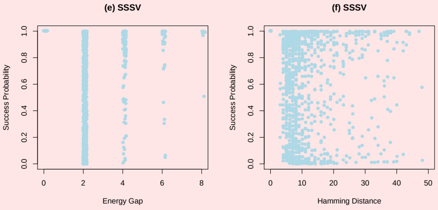

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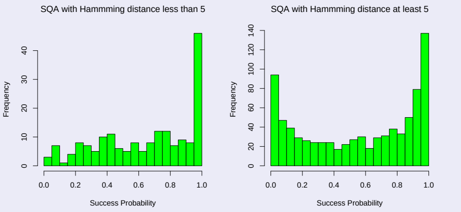

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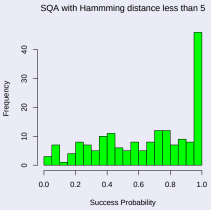

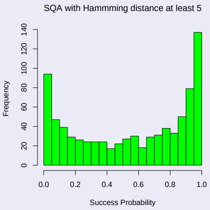

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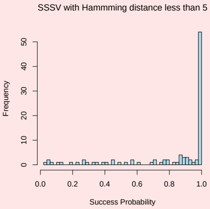

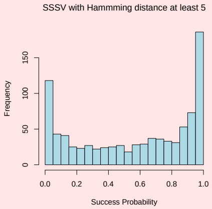

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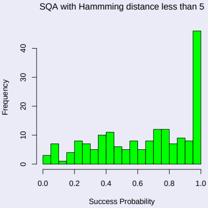
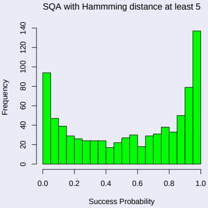
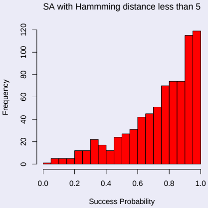
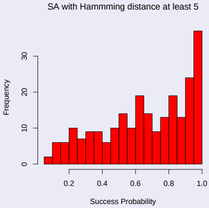
SQA



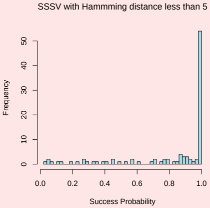


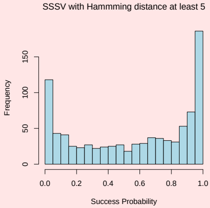
SA





SSSV





Concluding Remarks

Both inference and computing are inportant for big data.

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Both inference and computing are inportant for big data.

Interface

- Computing for conducting statistical inference; and statistics for analyzing computational algorithms.
- Statistics for quantum technology (e.g. quantum computing & tomography), and quantum computing for statistical computing and machine learning.